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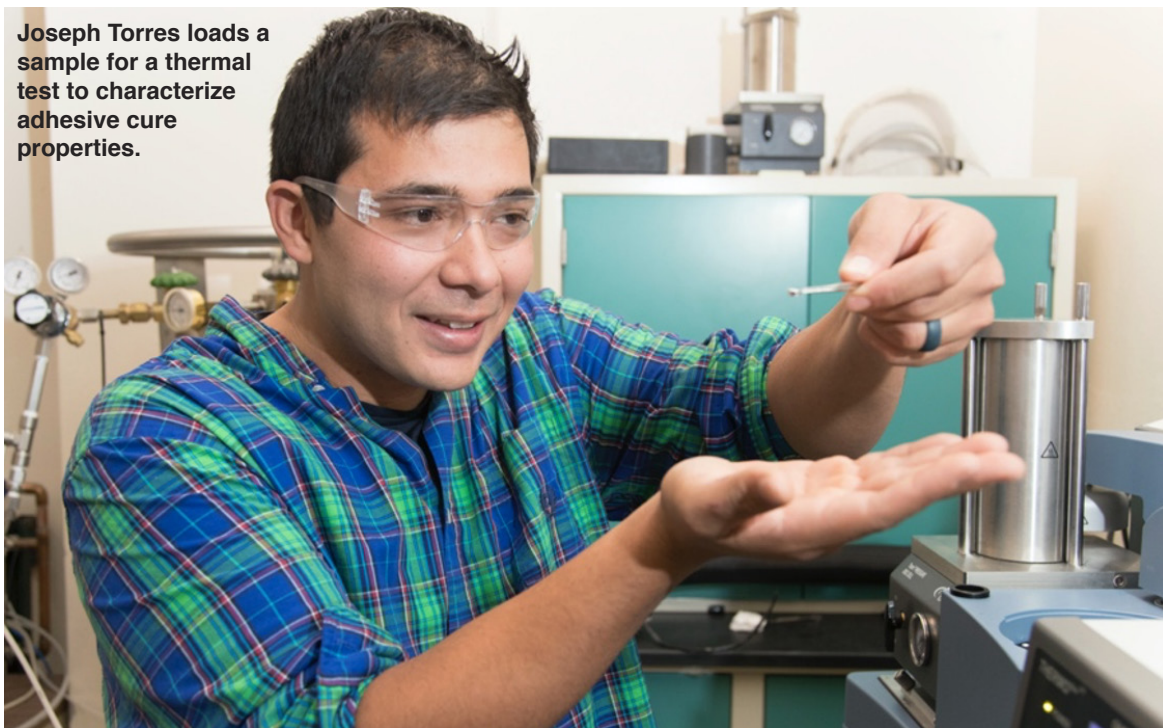
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Celebrating service

Joseph Torres loads a sample for a thermal test to characterize adhesive cure properties.



Joseph Torres



I enjoy being given a problem and developing a plan to attack that problem."

Mastering the art of the endgame in response to new and emerging national security threats

As a child, Joseph Torres learned to play chess from his father. The deliberate, focused game instilled in him at an early age the challenge of trying to solve a problem. To this day, he said, "I enjoy being given a problem and developing a plan to attack that problem."

Now, the research technologist on the Polymer Chemistry Team in Engineered Materials (MST-7) devises tactics to ensure future weapons systems are responsive to new and emerging threats. In particular, Torres focuses on developing materials and processes.

For example, he and his teammates are developing new material feedstocks for polymer powder bed additive manufacturing. This agility to print novel materials critical for many applications "will allow the weapons complex to be more responsive to future need," he said.

The task, Torres said, lies in the fact that available materials are typically limited to those offered by manufacturers. He and his teammates are employing creative methods that

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From Ellen's desk . . .

Dear MST,

It has a year of managing our work and deliverables while working to mitigate for the COVID hazard. I am pleased to say that because of your hard work, we have been able to achieve many of our deliverables, while learning how to adjust our work for COVID best practices. I know it hasn't been easy and all of us are tired, but vaccines are starting to be distributed, at an enhanced cadence both by the State and the Lab. And I think this will help as we consider our future.

With that said, some of the things that I put on hold last March as we tried to understand what COVID meant for our work and deliverables are activities in which we are starting to re-engage. One of the activities in which the MST management team has re-engaged is strategic planning. I know through your team meetings many of you were able to inform group-level documents that we are now using at the division level to develop this plan. The MST management team has met three times to establish a vision and mission statement for the division, a list of strengths and weaknesses, a list of critical factors for success, and finally a plan for what needs to be done to enable those success factors. Much of this was informed by the work you did at the team levels. In the upcoming weeks, the division intends to take this input and work with HR to draft a strategy that I hope to roll out to the division in April.

While I am by no means in a place to share even a draft document, I can comment on some of the emerging themes from our planning. Two that have my attention are: (1) infrastructure and space planning and (2) career development and recruitment. I was not surprised to see these themes emerge in our discussions about a strategic plan and also think that they are important enough that we can't wait until we have a finalized strategic plan to start working these issues. As such, your group offices and the division office have been actively engaged in a few activities that are specifically addressing, at least in part, these issues.

With regard to space and infrastructure two major efforts are in progress: (1) MST-7 and MST-16 management have been asked to work together to assemble a plan for a revitalized Target Fabrication Facility to consider expansion of Pu work in the facility, revitalization of cold lab space, and better use of space in general, and (2) MST, Sigma, and MPA have begun conversations to shape a new and refurbished materials campus at TA-3. If you have ideas with regard to these plans, please reach out to your group office.

With regard to career development, I have been trying to do a few things. The first is that I have been trying to create more virtual opportunities to engage early career staff. One event that I think was fairly successful was the MST and T Division event with division leaders. I was really pleased to see how many postdocs attended, so I am working with T Division to organize the next event. Another virtual opportunity that I want to direct everyone's attention to are the Virtual Coffees. A recent one was dedicated to a panel discussion featuring some of our established staff members in the division, who spoke about their career paths and how they got to where they are now. I am hopeful that the chance to hear about these diverse set of career paths inspires staff to consider the next steps in their own careers. Secondly, I have been working with HR and ALDPS to shape a new training for RLMs. The recent culture survey indicated that RLM training is desired and so I am hopeful there will be some new opportunities for those who are already RLMs as well as those who think they might want to be an RLM.

I realize that these efforts are just scratching the surface of the work that needs to be done, but I am optimistic that we can start to chip away at the issues of concern for the division and provide some appealing solutions for staff. As you consider your own work and input on the division strategic plan as well as what I have mentioned above, do not hesitate to reach out with your ideas and concerns—as you will likely shape my thinking on these topics.

Stay safe,
Ellen ■

“

As you consider your own work and input on the division strategic plan . . . do not hesitate to reach out with your ideas and concerns—as you will likely shape my thinking on these topics.

”

Torres cont.

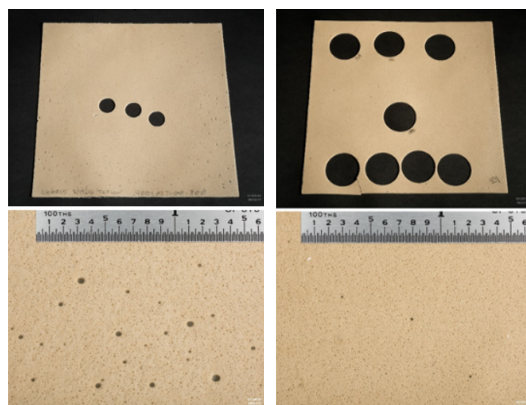
modify commercial, off-the-shelf powders and screen the formulations using a benchtop printer. Those formulations that meet mission demands will be printed using a production machine.

He and his teammates also work to improve legacy processes—those procedures that have been in place for decades and could be made better by applying current understanding and technology. For instance, traditional methods used for the past 50 years for mixing and pouring foams has been a hands-on, operator-dependent process that has poor historic yields. To improve manufacturability of the foam, a processing method has been identified that will automate the process and improve cell structure of the material (see photo). Torres is also collaborating with researchers at the Kansas City National Security Campus. Together they have established similar processing capabilities for the material and are sharing lessons learned and performing side-by-side studies to investigate its properties.

Torres joined the Lab in 2011 as a post-baccalaureate student, eager to expand on the research experience he gained while earning his bachelor's degree in chemistry at New Mexico Highlands University (NMHU).

As a student intern in MST-7, Torres was tasked with determining whether the pigments on an ancestral-Puebloan-period bowl were authentic. “Holding a piece of priceless history—hoping I did not drop it—was amazing,” he said. His spectroscopy measurements were critical in determining the composition of the pigments, enabling he and his colleagues to determine that the pottery was not a forgery.

Torres continues to hone the skills he learned at NMHU and later while earning his masters in chemistry from the Univer-



Visual appearance improvements: far left, hand-poured foam; left, machine-poured foam.

sity of Oregon. He employs them in projects that range from developing cutting-edge materials to characterizing polymer components in N95 masks and exploring the challenges of mask reuse.

“Joe has always been a problem solver—someone colleagues know they can count on to provide solutions,” said Team Leader Chris Hamilton, who has known Torres for a decade. “I have been enormously gratified to witness just how far Joe has come and how much he has grown. Joe manages several projects and he always delivers. He’s now leading multi-laboratory programs and, as a mentor, is second to none.”

Indeed, as a LANL student-turned-staffer, Torres takes a special interest in seeing that others have the opportunities he was given. For his work in mentoring students in his group, he received a 2018 Laboratory Distinguished Mentor Award. “That was definitely a highlight of working at LANL,” he said. “The opportunity to guide and aid in the development of students’ careers is rewarding and one of my passions.”

By Karen Kippen, ALDPS ■

Joseph Torres's favorite experiment

What: Optimizing processing parameters for an additive manufacturing (AM) process (selective laser sintering).

Why: Optimizing parameters such as energy density allows us to tailor the response of the final component to the component requirements. For instance, a part that maximizes dimensional stability may require different processing parameters compared with a part that maximizes strength. Ultimately, understanding processing parameters allows us to have more control of final part properties.

When: I have been working with this AM process since 2015. We are currently still optimizing processing parameters for new materials. Our team is always learning.

Where: Luckily, MST-7 has a production level machine at the Target Fabrication Facility. We have expanded our capabilities to include benchtop printers that increase productivity.

Who: We have a large team that supports the development of the AM process: Rachel Collino, Cade Willis, Anthony Sanchez, Estevan Sandoval, Natasha Story, Michael Garcia, and Jack Brett.

How: Initially, there was a learning curve to really understand certain parameters. AM platforms are typically “locked down” and offer very little control of parameters. Now the market has matured and manufacturers are allowing users to have more control. As a result, there was a lot of trial and error associated with the initial optimization.

The “a-ha” moment: The initial “a-ha” moment was when we started to change certain parameters and see real differences in the mechanical responses of the printed component.

From atoms to pins

Leveraging multiscale simulations to predict fission gas release from advanced nuclear fuel

As part of work carried out under the DOE Office of Nuclear Energy Advanced Modeling and Simulation (NEAMS) program, two key objectives in the modeling of traditional UO_2 and advanced UO_2 nuclear fuel concepts have been recently achieved: i) a cluster dynamics model was used to reproduce the experimentally observed irradiation-enhanced xenon diffusivity in UO_2 for the first time, and ii) the model was then applied to Cr_2O_3 -doped UO_2 to develop a mechanistic fission gas behavior model.

To enable useful predictions of nuclear fuel behavior beyond traditional operating envelopes, a mechanistic model based on fundamental phenomena is required. While a multiscale approach toward these problems—and in particular fission gas diffusion—is typically required, atomic-scale simulations often have trouble providing quantitative agreement with experimental measurements.

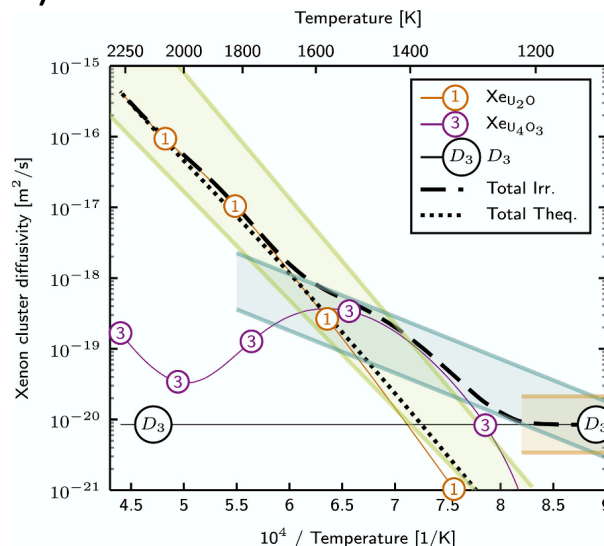
By integrating a wealth of density-functional-theory data developed at LANL with a newly published LANL cluster dynamics code, “Centipede,” the full spectrum of fission gas behavior across all expected temperatures and dose rates can now be mechanistically computed for the first time in UO_2 (see Figure A). This code predicts the diffusivities of dozens of xenon-containing defects in UO_2 , and most importantly the dominant large xenon clusters that drive irradiation enhanced diffusion. A critical aspect of the new cluster dynamics model is the use of the oxygen potential of the fuel as an input.

Unlike traditional UO_2 , there is limited experimental data of xenon diffusivity in Cr_2O_3 -doped UO_2 , posing a challenge to the development of new nuclear fuel performance modeling capability. To enable application of Centipede to doped UO_2 , it was first established, using thermodynamics calculations, that additions of Cr_2O_3 to UO_2 result in a two-phase Cr - Cr_2O_3 equilibrium that controls the oxygen potential. Implementation of this oxygen potential in Centipede shifts the stability of all point defects and clusters in the system, resulting in an enhancement in xenon diffusivity.

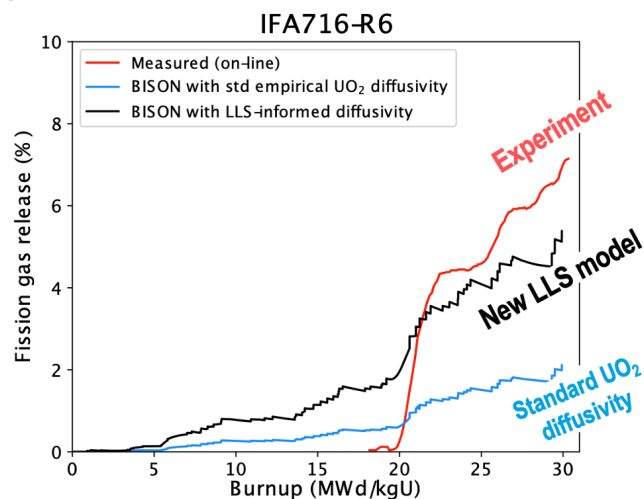
Los Alamos researchers, in collaboration with partners at Idaho National Laboratory (INL) and the Massachusetts Institute of Technology (MIT), used fuel performance simulations of fission gas release, which revealed that by including both enhanced diffusivity—as predicted by lower length scale simulations—and the large grains exhibited by Cr_2O_3 -doped UO_2 , a much-improved agreement with Halden Reactor test results is obtained (see Figure B). This work was recently published in two articles in the *Journal of Nuclear Materials*.

Traditional UO_2 : C. Matthews (Materials Science in Radiation and Dynamics Extremes, MST-8), R. Perriot (Physics and Chemistry of Materials, T-1), M.W.D. Cooper, C.R. Stanek, and D.A. Andersson (all MST-8), “Cluster dynamics simulation of xenon diffusion during irradiation in UO_2 ,” *Journal of Nuclear Materials* 540 152326 (2020).

A)



B)



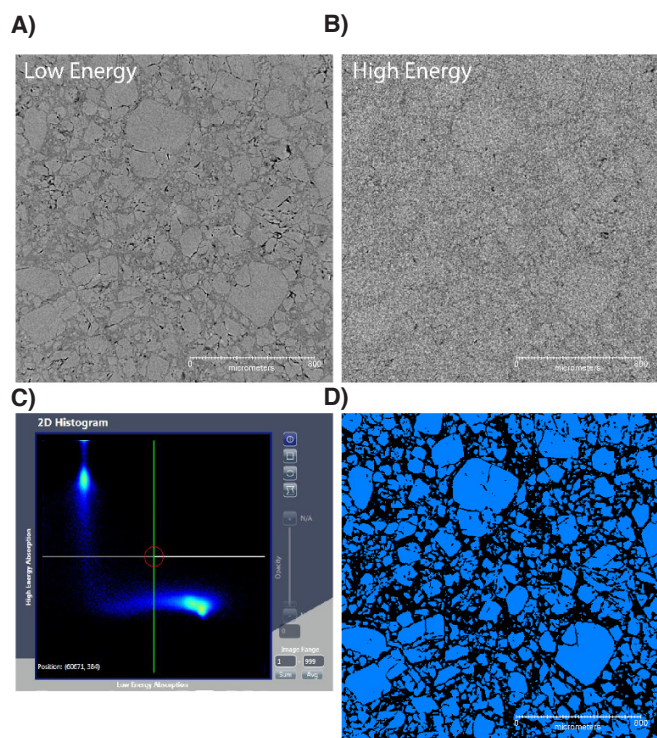
A) Cluster dynamics simulations of fission gas diffusivity in traditional UO_2 (lines) with comparison to experiment (colored bands) and B) demonstration of the new model for fission gas diffusivity in doped UO_2 for Bison simulations of fission gas release during a Halden Reactor Project test.

Doped UO_2 : M.W.D. Cooper (MST-8), G. Pastore (INL), Y. Che (MIT), C. Matthews (MST-8), A. Forslund (KTH Royal Institute of Technology, Sweden), C.R. Stanek (MST-8), K. Shivan (MIT), T. Tverberg (Institute for Energy Technology, Norway), K.A. Gamble (INL), B. Mays (Framatome Inc.), and D.A. Andersson (MST-8), “Fission gas diffusion and release for Cr_2O_3 -doped UO_2 : from the atomic to the engineering scale,” *Journal of Nuclear Materials* 545 152590 (2021). ■

Imaging breakthrough of plastic-bonded explosives

A team of researchers in MST-7 (Engineered Materials) and Q-5 (High Explosives Science and Technology) have been working to develop new three-dimensional (3D) x-ray imaging techniques and have created a library of 3D images of 10 different high explosive (HE) formulations. Plastic-bonded explosives (PBX) are comprised of an explosive crystal (e.g., HMX, TATB, or RDX) mixed into a polymer binder (e.g., Estane, HTPB, Kel-F, or viton A). Because the composition of both of these materials is primarily carbon, hydrogen, and oxygen, and the nearly identical mass density between the materials, the x-ray contrast within these materials is often negligible.

Due to these issues, segmentation and image analysis (i.e., differentiating between the crystals and the binder and then measuring the crystal distributions) is nearly impossible. In work recently published in *Materials*, the team describes use of a dual-energy x-ray imaging technique to better differentiate between the HE crystals and the surrounding binder. This technique collects a low x-ray energy 3D image as well as a high x-ray energy 3D image. The two images rely on the difference in absorption processes between the photoelectric effect at low energies and Compton scattering at higher energies. The images are then combined and a correlation plot between them is created. From this, correlation “hot-spots” are used to segment the material and differentiate between the crystals, binders, and voids. The figure below shows the low (A) and high (B) energy images, correlation plot (C), and a segmented image (D) of the crystals within a PBX 9501 specimen.



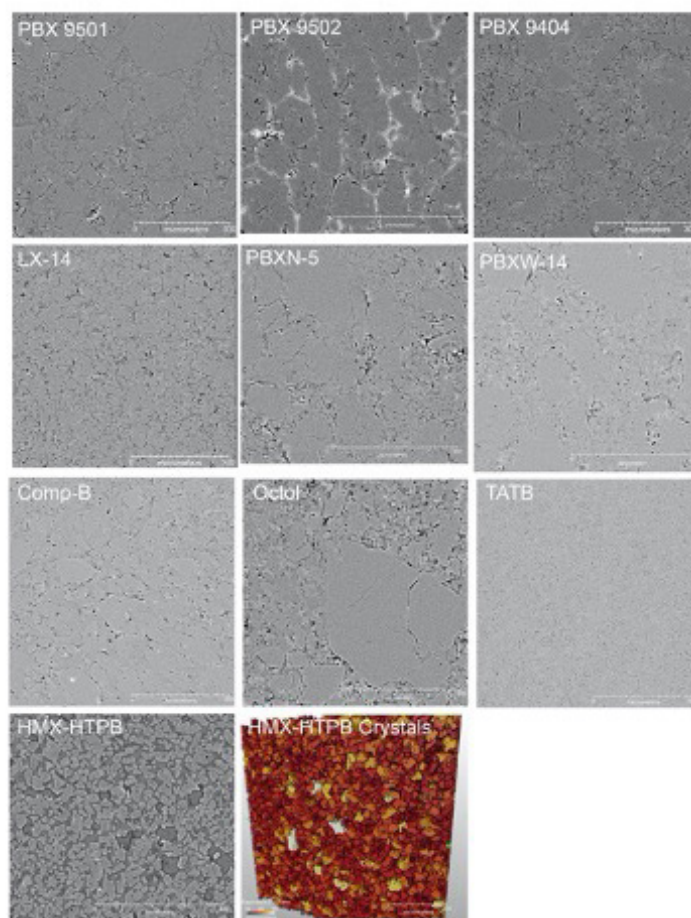
A single reconstructed slice from the dual-energy images low (A) and high (B). Correlation plot of the absorption values (C) and segmented image of the crystals (D) by the selection of one of the correlation “hot-spots.”

Additionally, the team has been working to create a library of high-resolution 3D tomographic images of the 10 most commonly LANL-studied HE materials. These include: HMX-HTPB, PBX 9501, PBX 9502, PBX 9404, LX-14, PBXN-5, PBXW-14, Composition B, Octol, and TATB. Each of these materials were imaged with $\sim 0.8 \mu\text{m}$ voxel size. The figure below shows a single reconstructed slice of the ~ 2000 collected to make the 3D data set for these materials as well as a 3D rendering of the individual HMX crystals within the HMX-HTPB formulation. These high-resolution 3D images of the PBX microstructure are available to researchers. Most were also imaged with the aforementioned dual-energy modality for modeling or other uses.

Team members are Brian M. Patterson, Lindsey Kuettner (MST-7); John D. Yeager, Amanda L. Duque, and Larry G. Hill (Q-5). The work was supported by Delivery Environments (LANL Program Manager Antranik Siranosian) and Campaign 2 (LANL program Dana Dattelbaum).

Reference: “Microcomputed x-ray tomographic imaging and image processing for microstructural characterization of explosives,” *Materials* 13, 20 (2020).

Technical contacts: John D. Yeager and Brian M. Patterson ■



Individual reconstructed slices for each of the 10 formulations and a 3D rendering of the HMX-HTPB. Crystals are colored by their size.

MST news roundup

Saryu Fensin joins APR early career editorial board

Saryu Fensin (Materials Science in Radiation and Dynamics Extremes, MST-8) has joined the Early Career Editorial Advisory Board of *Applied Physics Reviews*. Her three-year term began in January. Fensin, who earned her PhD in materials science and engineering from the University of California, Davis, is a member of MST-8's Dynamic and Quasi-Static Loading (experimental) team. ■



MST staff elected to ACS local section leadership positions

Dom Peterson (Materials Science and Technology, MST-DO) was elected a national councilor for the Central New Mexico Local Section of the American Chemical Society (ACS). For three years he will represent the section at national council meetings held twice yearly. He will also participate in committees representing various interest groups among the ACS membership.

Alex Edgar (Engineered Materials, MST-7) was elected 2021 chair elect and will serve as 2022 chair and 2023 post chair. He will facilitate regional meetings and host several public events sponsored by the local section.

Dali Yang (MST-7) was reelected advisor to the local section. She will participate in public events and as a voting member in any discussion by the executive board of the local section. ■

History of plutonium metallurgy to be published

"The taming of plutonium: Pu metallurgy and the Manhattan Project" (LA-UR-21-20337), written by Joe Martz (Materials Science and Technology, MST-DO), and Franz Freibert and David Clark (both National Security Education Center, NSEC), is set to be published in *Weapon Review Letters* and a special issue of the *ANS Journal*.

Many details are described for the first time in a journal publication. For example, the paper contains a listing of the initial alloys attempted during the Manhattan Project in a search to find a suitable delta-stabilizer, the first time such a comprehensive description is provided in a single table. ■

HeadsUP!

Mexican spotted owl protections in effect through August

Beginning March 1, LANL stopped the use of heavy work equipment in habitats of Mexican spotted owls.

The restrictions are part of the Lab's Habitat Management Plan, an agreement between the DOE, NNSA, and the U.S. Fish and Wildlife Service that explains what the Lab does to protect habitats that are threatened or endangered.

As part of the plan, certain activities—such as heavy equipment work in canyons—are subject to annual seasonal restrictions.

Restrictions will be applied through Aug. 31 if endangered species' habitats are identified. If there are no endangered habitats in the given area, restrictions could be lifted as early as May.

If you're a contractor, subcontractor, or employee who works in a seasonally restricted area, take a look at the biological comments in your PR-ID and/or EX-ID comments in the Integrated Review Tool.

Celebrating service

Congratulations to the following MST Division employees who recently celebrated a service anniversary:

Lynne Goodwin, MST-7	30 years
James Valdez, MST-8	25 years
Rodney McCabe, MST-8	20 years
Blas Uberuaga, MST-8	20 years
Sven Vogel, MST-8	20 years
Alice Smith, MST-16.....	15 years
Christopher Cordova, MST-16	5 years
Amber Telles, MST-8.....	5 years

MSTe NEWS

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To submit news items or for more information, contact Karen Kippen, ALDPS Communications, at 505-606-1822 or aldps-comm@lanl.gov.

For past issues, see www.lanl.gov/org/ddste/aldps/mst-e-news.php.



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